

Exact ground states of frustrated quantum spin systems consisting of spin-dimer units

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We study frustrated quantum spin systems consisting of dimers of spin-1/2 spins. We derive several models which have the exact ground state of the form of the direct product of dimer states. The ground states realized include the product state of dimer-singlets, that of dimer-triplets with zero magnetization, those of dimer-spin-nematic states, and those of a mixture of the dimer states. Pseudo spin-1/2 operators emerging in each dimers are also introduced.

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I. INTRODUCTION

Frustrated magnetism has been one of the central issues in condensed-matter physics for several decades. In frustrated magnets, a competition among interactions leads to a massive degeneracy in the ground-state manifold and provides a good opportunity for perturbations such as the quantum fluctuation to realize an unconventional ground state. Studies searching for such an unconventional ground state in frustrated quantum magnets have been performed intensively and succeeded to identify exotic ground states, *e.g.*, the quantum spin-liquid in Kagomé antiferromagnet¹⁻⁴, the vector-chirality state in the quantum magnets in zigzag ladder⁵⁻¹², and the spin-multipolar state in low-dimensional frustrated ferromagnets¹³⁻¹⁶.

Despite of the efforts made for many years, studying frustrated quantum magnets is still a challenging task. This is mainly due to the fact that many powerful theoretical tools to investigate quantum spin systems are not applicable to the problem. For instance, the mean-field approximation is not justified in investigating unconventional states without a classical long-range order. The quantum Monte-Carlo method breaks down when applied to frustrated systems because of the notorious negative-sign problem. Therefore, accurate results, especially exact ones, for the frustrated quantum magnets are highly desirable.

A famous example of frustrated quantum spin models having the exact ground state is the Majumdar-Ghosh model^{17,18}. The model has a form of zigzag spin ladder and is constructed as a sum of projection operators. It was then shown that the model has the product states of singlet pairs of nearest-neighbor spins as the ground state with a finite excitation gap. Exact ground states having the form of the product of local-spin-unit states have also been reported for various frustrated models¹⁹⁻²⁶.

In this work, we discuss frustrated quantum spin systems which consist of dimers of spin-1/2 spins and have a product state of the dimer states as an exact ground state. The model Hamiltonian is composed of the inter- and intra-dimer parts,

$$\mathcal{H} = \mathcal{H}_{\text{inter}} + \mathcal{H}_{\text{intra}}. \quad (1)$$

The inter-dimer Hamiltonian consists of the XXZ exchange

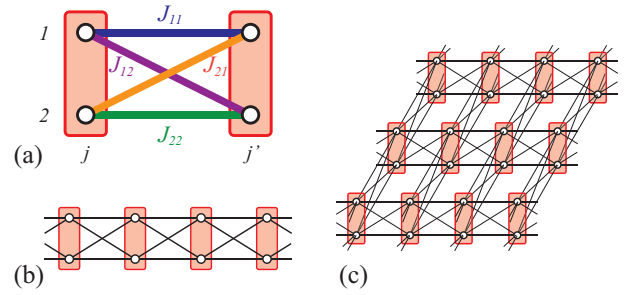


FIG. 1: (a) Schematic picture of inter-dimer exchange couplings. Rectangles and circles represent dimer units and spin-1/2 spins, respectively. Solid lines represent inter-dimer XXZ exchange couplings. (b) System in one-dimensional lattice. (c) System in two-dimensional square lattice.

couplings,

$$\begin{aligned} \mathcal{H}_{\text{inter}} &= \sum_{\langle j, j' \rangle} h^{\text{inter}}(j, j') \\ &= \sum_{\langle j, j' \rangle} \left[J_{11}(\mathbf{S}_{1,j}, \mathbf{S}_{1,j'})_{\Delta} + J_{22}(\mathbf{S}_{2,j}, \mathbf{S}_{2,j'})_{\Delta} \right. \\ &\quad \left. + J_{12}(\mathbf{S}_{1,j}, \mathbf{S}_{2,j'})_{\Delta} + J_{21}(\mathbf{S}_{2,j}, \mathbf{S}_{1,j'})_{\Delta} \right], \quad (2) \end{aligned}$$

where $\mathbf{S}_{n,j} = (S_{n,j}^x, S_{n,j}^y, S_{n,j}^z)$ ($n = 1, 2$) are spin-1/2 operators in the j th dimer and $(\mathbf{S}_{n,j}, \mathbf{S}_{n',j'})_{\Delta}$ represents the XXZ anisotropic exchange coupling, *i.e.*,

$$(\mathbf{S}_{n,j}, \mathbf{S}_{n',j'})_{\Delta} = S_{n,j}^x S_{n',j'}^x + S_{n,j}^y S_{n',j'}^y + \Delta S_{n,j}^z S_{n',j'}^z. \quad (3)$$

A schematic picture of the inter-dimer Hamiltonian is shown in Fig. 1(a). We note that the exchange constants J_{11} , J_{22} , J_{12} , and J_{21} are different in general while we consider the case where the anisotropy parameter Δ is the same for all the inter-dimer couplings. The sum $\sum_{\langle j, j' \rangle}$ in Eq. (2) is taken for all the bonds connected by the inter-dimer exchange couplings. [See Figs. 1(b) and (c) for example.] The structure of the lattice composed of the inter-dimer exchanges is basically arbitrary; a major part of our results is valid for any lattice in any dimension while for some results we require that the lattice is bipartite.

For the intra-dimer Hamiltonian, we consider the XXZ and further anisotropic exchange couplings²⁷, the Dzyaloshinskii-Moriya (DM) coupling with the DM vector in the z -direction, and the Zeeman terms of uniform and staggered fields. The intra-dimer Hamiltonian is then given by

$$\begin{aligned}\mathcal{H}_{\text{intra}} &= \sum_j h_{\text{intra}}(j) \\ &= \sum_j \left[h^{XXZ}(j) + h^{\text{ani}}(j) + h^{\text{DM}z}(j) \right. \\ &\quad \left. + h^{\text{uni}}(j) + h^{\text{sg}}(j) \right],\end{aligned}\quad (4)$$

$$h^{XXZ}(j) = J_d(j)(S_{1,j}, S_{2,j})_{\Delta_d(j)}, \quad (5)$$

$$h^{\text{ani}}(j) = K_d(j) \left[e^{i\eta_d(j)} S_{1,j}^+ S_{2,j}^+ + e^{-i\eta_d(j)} S_{1,j}^- S_{2,j}^- \right], \quad (6)$$

$$h^{\text{DM}z}(j) = D_d(j)(S_{1,j} \times S_{2,j})^z, \quad (7)$$

$$h^{\text{uni}}(j) = -H_d^{\text{uni}}(j)(S_{1,j}^z + S_{2,j}^z), \quad (8)$$

$$h^{\text{sg}}(j) = -H_d^{\text{sg}}(j)(S_{1,j}^z - S_{2,j}^z), \quad (9)$$

where $S_{n,j}^\pm = S_{n,j}^x \pm iS_{n,j}^y$. The parameters in the intra-dimer Hamiltonian can change depending on the dimer position j in general, but we will mainly discuss the case where they are uniform or the case where they respectively take one of two values depending on the sublattice, to which the dimer belongs, in a bipartite lattice.

We prove that the model (1) in certain parameter regimes has an exact ground state which is described by a direct product of dimer states [see Eqs. (19) and (20) for the definitions]. The dimer states can be the superposition of $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$ or that of $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$, where $|\sigma_1\sigma_2\rangle_j$ represents the dimer state in which the state of the spin $S_{n,j}$ is $\sigma_n = \uparrow, \downarrow$ ($n = 1, 2$); the dimer states include the spin-singlet state of the two spins in the dimer unit, the triplet state with zero magnetization, and the spin-nematic states. The key idea in the proof is to show that the product state considered is an eigenstate of the inter-dimer Hamiltonian with zero eigenvalue²⁵. Then, if the product state is simultaneously the lowest-energy eigenstate of intra-dimer Hamiltonian and the energy gap to the first excited states is sufficiently large, the product state, which is not disturbed by the inter-dimer Hamiltonian, remains the ground state even when the inter-dimer Hamiltonian is added to the intra-dimer Hamiltonian. In such a manner, we derive several models and their exact ground states.

The paper is organized as follows. In Sect. II, we develop pseudo spin-1/2 operators composed of the two spin-1/2 spins in a dimer unit, which are used in the following argument. The product states considered are also defined. Our results of the exact ground state are presented in Sect. III. We discuss the construction of the inter-dimer Hamiltonian having the product states as eigenstates with zero eigenvalue in Sect. III A, and then, provide several examples of the model having the exact ground state in Sects. III B - III D. Section IV contains a summary of our results.

II. PSEUDO-SPIN OPERATORS AND PRODUCT STATES

In this section, we introduce two pseudo spin-1/2 operators defined in each dimer unit, which are used in the following discussion. The wave functions which have the form of the direct product of dimer states and will be considered as candidates of the exact ground state are also defined.

Let us focus on the spins $S_{1,j}$ and $S_{2,j}$ in a dimer unit. We construct two operators $T_{1,j}$ and $T_{2,j}$ defined by

$$T_{1,j}^z = \frac{1}{2}(S_{1,j}^z - S_{2,j}^z), \quad T_{1,j}^\pm = S_{1,j}^\pm S_{2,j}^\mp, \quad (10)$$

$$T_{2,j}^z = \frac{1}{2}(S_{1,j}^z + S_{2,j}^z), \quad T_{2,j}^\pm = S_{1,j}^\pm S_{2,j}^\pm. \quad (11)$$

One can easily find that these operators obey the following commutation relations,

$$[T_{1,j}^\alpha, T_{1,j}^\beta] = i\epsilon^{\alpha\beta\gamma} T_{1,j}^\gamma, \quad (12)$$

$$[T_{2,j}^\alpha, T_{2,j}^\beta] = i\epsilon^{\alpha\beta\gamma} T_{2,j}^\gamma, \quad (13)$$

$$[T_{1,j}^\alpha, T_{2,j}^\beta] = 0, \quad (14)$$

where $T_{n,j}^x = (T_{n,j}^+ + T_{n,j}^-)/2$, $T_{n,j}^y = (T_{n,j}^+ - T_{n,j}^-)/(2i)$, and $\epsilon^{\alpha\beta\gamma}$ is the Levi-Civita symbol. The operators $T_{1,j}$ and $T_{2,j}$ thus satisfy the usual commutation relations of spin operators and commute with each other. Furthermore, actions of the operator $T_{1,j}$ on the dimer states are found as

$$\begin{aligned}T_{1,j}^z |\uparrow\downarrow\rangle_j &= \frac{1}{2} |\uparrow\downarrow\rangle_j, \quad T_{1,j}^z |\downarrow\uparrow\rangle_j = -\frac{1}{2} |\downarrow\uparrow\rangle_j, \\ T_{1,j}^+ |\uparrow\downarrow\rangle_j &= 0, \quad T_{1,j}^+ |\downarrow\uparrow\rangle_j = |\uparrow\downarrow\rangle_j, \\ T_{1,j}^- |\uparrow\downarrow\rangle_j &= |\downarrow\uparrow\rangle_j, \quad T_{1,j}^- |\downarrow\uparrow\rangle_j = 0, \\ T_{1,j}^\alpha |\uparrow\uparrow\rangle_j &= T_{1,j}^\alpha |\downarrow\downarrow\rangle_j = 0. \quad (\alpha = x, y, z)\end{aligned}\quad (15)$$

Therefore, $T_{1,j}$ behaves as a pseudo spin-1/2 operator in the subspace $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$. The states $|\uparrow\downarrow\rangle_j$ and $|\downarrow\uparrow\rangle_j$ corresponds to the states $|T_{1,j}^z = 1/2\rangle_j$ and $|T_{1,j}^z = -1/2\rangle_j$, respectively. In the subspace $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$, $T_{1,j}$ is zero. Similarly, it is found that $T_{2,j}$ behaves as a pseudo spin-1/2 operator in the subspace $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$ with $|\uparrow\uparrow\rangle_j = |T_{2,j}^z = 1/2\rangle_j$ and $|\downarrow\downarrow\rangle_j = |T_{2,j}^z = -1/2\rangle_j$, while $T_{2,j}$ is zero in the subspace $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$. We note that the construction of the operators $T_{1,j}$ and $T_{2,j}$ from the original spin operators $S_{1,j}$ and $S_{2,j}$ has the same structure as that of the spin and η operators from fermion operators^{28,29}.

Next, we consider a unitary transformation for dimer states,

$$U_j(\theta_j, \chi_j; \varphi_j, \zeta_j) = U_{1,j}(\theta_j, \chi_j) U_{2,j}(\varphi_j, \zeta_j), \quad (16)$$

with

$$U_{1,j}(\theta_j, \chi_j) = \exp(-i\chi_j T_{1,j}^z) \exp(-i\theta_j T_{1,j}^y), \quad (17)$$

$$U_{2,j}(\varphi_j, \zeta_j) = \exp(-i\zeta_j T_{2,j}^z) \exp(-i\varphi_j T_{2,j}^y), \quad (18)$$

which represent the rotation of the pseudo spins $T_{1,j}$ and $T_{2,j}$, respectively. Note that $U_{1,j}(\theta_j, \chi_j)$ and $U_{2,j}(\varphi_j, \zeta_j)$ are commute with each other and $U_{1,j}(\theta_j, \chi_j) [U_{2,j}(\varphi_j, \zeta_j)]$ is an identity operator in the subspace $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$ [$|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j$].

$\rangle_j]$. Using these transformations, we introduce the following dimer states,

$$\begin{aligned} |\psi(\theta_j, \chi_j)\rangle_j &= U_{1,j}(\theta_j, \chi_j) |\uparrow\downarrow\rangle_j \\ &= e^{-i\frac{\chi_j}{2}} \cos\left(\frac{\theta_j}{2}\right) |\uparrow\downarrow\rangle_j + e^{i\frac{\chi_j}{2}} \sin\left(\frac{\theta_j}{2}\right) |\downarrow\uparrow\rangle_j, \end{aligned} \quad (19)$$

$$\begin{aligned} |\phi(\varphi_j, \zeta_j)\rangle_j &= U_{2,j}(\varphi_j, \zeta_j) |\uparrow\uparrow\rangle_j \\ &= e^{-i\frac{\zeta_j}{2}} \cos\left(\frac{\varphi_j}{2}\right) |\uparrow\uparrow\rangle_j + e^{i\frac{\zeta_j}{2}} \sin\left(\frac{\varphi_j}{2}\right) |\downarrow\downarrow\rangle_j. \end{aligned} \quad (20)$$

We take the ranges of the phases as $0 \leq \theta_j < 2\pi$, $0 \leq \chi_j \leq \pi$, $0 \leq \varphi_j < 2\pi$, and $0 \leq \zeta_j \leq \pi$. In terms of the pseudo-spin operators, $|\psi(\theta_j, \chi_j)\rangle_j$ [$|\phi(\varphi_j, \zeta_j)\rangle_j$] corresponds to the state of $T_{1,j}$ [$T_{2,j}$] pointing to the direction $(T_{1,j}^x, T_{1,j}^y, T_{1,j}^z) = (\sin\theta_j \cos\chi_j, \sin\theta_j \sin\chi_j, \cos\theta_j)$ [$(T_{2,j}^x, T_{2,j}^y, T_{2,j}^z) = (\sin\varphi_j \cos\zeta_j, \sin\varphi_j \sin\zeta_j, \cos\varphi_j)$]. We note that the four

states $\{|\psi(\theta_j, \chi_j)\rangle_j, |\psi(\theta_j + \pi, \chi_j)\rangle_j, |\phi(\varphi_j, \zeta_j)\rangle_j, |\phi(\varphi_j + \pi, \zeta_j)\rangle_j\}$ are orthogonal to each other and therefore can be used as an orthonormal basis for the dimer states.

Finally, it is instructive to note that the intra-dimer coupling terms Eqs.(5) - (9) are rewritten in terms of the operators $T_{1,j}$ and $T_{2,j}$ as

$$h^{XXZ}(j) = J_d(j)T_{1,j}^x + J_d(j)\Delta_d(j) \left[2(T_{2,j}^z)^2 - \frac{1}{4} \right], \quad (21)$$

$$h^{\text{ani}}(j) = 2K_d(j) \{ \cos[\eta_d(j)]T_{2,j}^x - \sin[\eta_d(j)]T_{2,j}^y \}, \quad (22)$$

$$h^{\text{DMz}}(j) = -D_d(j)T_{1,j}^y, \quad (23)$$

$$h^{\text{uni}}(j) = -2H_d^{\text{uni}}(j)T_{2,j}^z, \quad (24)$$

$$h^{\text{stg}}(j) = -2H_d^{\text{stg}}(j)T_{1,j}^z. \quad (25)$$

The intra-dimer Hamiltonian (4) has a block-diagonal form,

$$h_{\text{intra}}(j) = \begin{pmatrix} -\frac{1}{4}J_d(j)\Delta_d(j) - H_d^{\text{stg}}(j) & \frac{1}{2}J_d(j) + \frac{i}{2}D_d(j) & 0 & 0 \\ \frac{1}{2}J_d(j) - \frac{i}{2}D_d(j) & -\frac{1}{4}J_d(j)\Delta_d(j) + H_d^{\text{stg}}(j) & 0 & 0 \\ 0 & 0 & \frac{1}{4}J_d(j)\Delta_d(j) - H_d^{\text{uni}}(j) & K_d(j)e^{i\eta_d(j)} \\ 0 & 0 & K_d(j)e^{-i\eta_d(j)} & \frac{1}{4}J_d(j)\Delta_d(j) + H_d^{\text{uni}}(j) \end{pmatrix}, \quad (26)$$

where the basis kets are arranged in the order of $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j, |\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$. Therefore, the eigenstates of the intra-dimer Hamiltonian $h_{\text{intra}}(j)$ for each dimer can be expressed as $\{|\psi(\theta_{0j}, \chi_{0j})\rangle_j, |\psi(\theta_{0j} + \pi, \chi_{0j})\rangle_j, |\phi(\varphi_{0j}, \zeta_{0j})\rangle_j, |\phi(\varphi_{0j} + \pi, \zeta_{0j})\rangle_j\}$. The phases θ_{0j} , χ_{0j} , φ_{0j} , and ζ_{0j} are determined as functions of the coupling constants in $h_{\text{intra}}(j)$. These results about the intra-dimer Hamiltonian $h_{\text{intra}}(j)$ will be used in Sect. III to obtain the exact ground state of the model (1).

III. EXACT GROUND STATE

In this section, we show our main result that the model (1) in some parameter regions has an exact ground state of the form of the direct product of dimer states. The strategy used to prove the result is as follows.

- (i) We first focus on the inter-dimer Hamiltonian (2) in a certain parameter region and show that the Hamiltonian has the product states of the dimer states Eqs. (19) and (20) with some constraints on the phases $\{\theta_j, \chi_j, \varphi_j, \zeta_j\}$ as eigenstates with zero eigenvalue.
- (ii) We show that the product states with additional constraints on the phases are the eigenstates of the intra-dimer Hamiltonian (4) considered. At this stage, the product states obtained turn out to be eigenstates of the whole Hamiltonian (1).

- (iii) Finally, we specify the parameter region of the intra-dimer Hamiltonian which lowers the eigenenergy of one of the eigenstates obtained in (ii) and make it be the ground state of the whole Hamiltonian.

A. Inter-dimer Hamiltonian

Let us consider the inter-dimer exchange Hamiltonian $h^{\text{inter}}(j, j')$ [Eq. (2)] between the dimers (j, j') . Here, we rewrite the Hamiltonian as

$$h^{\text{inter}}(j, j') = \sum_{\epsilon, \epsilon' = \pm} \tilde{J}_{\epsilon\epsilon'} \left[h_{\epsilon\epsilon'}^{\text{XY}}(j, j') + \Delta h_{\epsilon\epsilon'}^{\text{Ising}}(j, j') \right], \quad (27)$$

with

$$h_{\epsilon\epsilon'}^{\text{XY}}(j, j') = (S_{1,j}^x + \epsilon S_{2,j}^x)(S_{1,j'}^x + \epsilon' S_{2,j'}^x) + (S_{1,j}^y + \epsilon S_{2,j}^y)(S_{1,j'}^y + \epsilon' S_{2,j'}^y), \quad (28)$$

$$h_{\epsilon\epsilon'}^{\text{Ising}}(j, j') = (S_{1,j}^z + \epsilon S_{2,j}^z)(S_{1,j'}^z + \epsilon' S_{2,j'}^z). \quad (29)$$

The original coupling constants $\{J_{11}, J_{12}, J_{21}, J_{22}\}$ are related to $\tilde{J}_{\epsilon\epsilon'}$ as

$$\begin{aligned} J_{11} &= \tilde{J}_{++} + \tilde{J}_{+-} + \tilde{J}_{-+} + \tilde{J}_{--}, \\ J_{12} &= \tilde{J}_{++} - \tilde{J}_{+-} + \tilde{J}_{-+} - \tilde{J}_{--}, \\ J_{21} &= \tilde{J}_{++} + \tilde{J}_{+-} - \tilde{J}_{-+} - \tilde{J}_{--}, \\ J_{22} &= \tilde{J}_{++} - \tilde{J}_{+-} - \tilde{J}_{-+} + \tilde{J}_{--}. \end{aligned} \quad (30)$$

We consider the coupling terms $h_{\epsilon\epsilon'}^{XY}(j, j')$ and $h_{\epsilon\epsilon'}^{\text{Ising}}(j, j')$ acting on the following four product states of the two dimers, $|\psi(\theta_j, \chi_j)\rangle_j |\psi(\theta_{j'}, \chi_{j'})\rangle_{j'}$, $|\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$, $|\psi(\theta_j, \chi_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$, and $|\phi(\varphi_j, \zeta_j)\rangle_j |\psi(\theta_{j'}, \chi_{j'})\rangle_{j'}$. For the Ising terms, the calculation is simple since $h_{\epsilon\epsilon'}^{\text{Ising}}(j, j')$'s are expressed in terms of z components of the pseudo-spin operators such as $h_{++}^{\text{Ising}}(j, j') = 4T_{2,j}^z T_{2,j'}^z$ and so on. The operator $T_{1,k}^z$ [$T_{2,k}^z$] ($k = j, j'$) acting on the state $|\psi(\theta_k, \chi_k)\rangle_k$ [$|\phi(\varphi_k, \zeta_k)\rangle_k$] yields zero irrespective of (θ_k, χ_k) [(φ_k, ζ_k)]. The action of the XY terms $h_{\epsilon\epsilon'}^{XY}(j, j')$ on the states is a little complicated since the terms have matrix elements between the subspaces $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$ and $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$. However, we can obtain the resultant states by a straightforward calculation. Some details of the calculation are presented in Appendix. An interesting finding is that some of the resultant states with certain conditions on the phases $\{\theta_j, \chi_j, \theta_{j'}, \chi_{j'}\}$ or $\{\varphi_j, \zeta_j, \varphi_{j'}, \zeta_{j'}\}$ are zero. The conditions on the phases required for obtaining the zero state are summarized in Table I. Using the results in the table, we can construct the inter-dimer Hamiltonian $\mathcal{H}_{\text{inter}}$ [Eq. (2)] having exact eigenstates with zero eigenvalue. In the following sections, we discuss some typical examples of the inter-dimer Hamiltonian and show that the Hamiltonian combined with an appropriate intra-dimer Hamiltonian has an exact ground state.

B. Example I of exact ground states

Here, we consider the inter-dimer Hamiltonian of the form,

$$\mathcal{H}_{\text{inter}} = \sum_{(j,j')} \left\{ \tilde{J}_{+-} [h_{+-}^{XY}(j, j') + \Delta h_{+-}^{\text{Ising}}(j, j')] + \tilde{J}_{-+} [h_{-+}^{XY}(j, j') + \Delta h_{-+}^{\text{Ising}}(j, j')] \right\}. \quad (31)$$

This inter-dimer Hamiltonian corresponds to Eq. (2) with $J_{11} = -J_{22} = \tilde{J}_{+-} + \tilde{J}_{-+}$, $J_{21} = -J_{12} = \tilde{J}_{+-} - \tilde{J}_{-+}$ [see Fig. 2 (a)]. When $\tilde{J}_{+-} = \tilde{J}_{-+}$, the Hamiltonian is reduced to a simpler one, Eq. (2) with $J_{11} = -J_{22}$ and $J_{21} = J_{12} = 0$ [Fig. 2 (b)].

As seen in Table I, $h_{+-}^{XY}(j, j')$ and $h_{-+}^{XY}(j, j')$ acting on $|\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$ give zero for $\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$. The Ising terms $h_{+-}^{\text{Ising}}(j, j')$ and $h_{-+}^{\text{Ising}}(j, j')$ acting on the same state also yield zero irrespective of the phases. From these results, it follows that the product state for the whole system,

$$\prod_j |\phi(\varphi_j, \zeta_j)\rangle_j, \quad (32)$$

is an eigenstate of the model (31) with the zero eigenvalue when the phases φ_j and ζ_j are uniform, $\varphi_j = \varphi$ and $\zeta_j = \zeta$, for arbitrary φ and ζ . Similarly, it is found in Table I that $h_{+-}^{XY}(j, j') + h_{-+}^{XY}(j, j')$ acting on $|\psi(\theta_j, \chi_j)\rangle_j |\psi(\theta_{j'}, \chi_{j'})\rangle_{j'}$ with $\theta_j = \theta_{j'}$ and $\chi_j = \chi_{j'}$ as well as $h_{+-}^{\text{Ising}}(j, j') + h_{-+}^{\text{Ising}}(j, j')$ acting on the same state (with arbitrary $\{\theta_j, \chi_j, \theta_{j'}, \chi_{j'}\}$) yield zero. Therefore, if the relation $\tilde{J}_{+-} = \tilde{J}_{-+}$ holds, the product state,

$$\prod_j |\psi(\theta_j, \chi_j)\rangle_j, \quad (33)$$

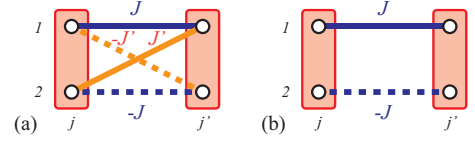


FIG. 2: Schematic pictures of (a) the inter-dimer Hamiltonian (31) where $J = \tilde{J}_{+-} + \tilde{J}_{-+}$ and $J' = \tilde{J}_{+-} - \tilde{J}_{-+}$, and (b) the same Hamiltonian with $\tilde{J}_{+-} = \tilde{J}_{-+}$.

with the uniform phases $\theta_j = \theta$ and $\chi_j = \chi$ is also an eigenstate of the model (31) with the zero eigenvalue for arbitrary θ and χ .

Next, we include the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ [Eq. (4)] in the argument. Here, we consider the case where the coupling constants in the intra-dimer Hamiltonian are uniform, i.e., $J_d(j) = J_d$, $\Delta_d(j) = \Delta_d$, and so on. As discussed in Sect. II, the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ has eigenstates $|\psi(\theta_0, \chi_0)\rangle_j$, $|\psi(\theta_0 + \pi, \chi_0)\rangle_j$, $|\phi(\varphi_0, \zeta_0)\rangle_j$, $|\phi(\varphi_0 + \pi, \zeta_0)\rangle_j$, where the phases $\theta_0, \chi_0, \varphi_0$, and ζ_0 are determined by the coupling constants. The phases are independent of the position j since the coupling constants are uniform. Combining this result with the one for the inter-dimer Hamiltonian discussed above, we find that the two product states $\prod_j |\phi(\varphi_j, \zeta_j)\rangle_j$ with $\varphi_j = \varphi_0, \varphi_0 + \pi$ and $\zeta_j = \zeta_0$ are eigenstates of the whole Hamiltonian $\mathcal{H}_{\text{inter}} + \mathcal{H}_{\text{intra}}$. Furthermore, if $\tilde{J}_{+-} = \tilde{J}_{-+}$, the other two product states $\prod_j |\psi(\theta_j, \chi_j)\rangle_j$ with $\theta_j = \theta_0, \theta_0 + \pi$ and $\chi_j = \chi_0$ are also eigenstates of the whole Hamiltonian.

We note that when the eigenstates $|\psi(\theta_0, \chi_0)\rangle_j$ and $|\psi(\theta_0 + \pi, \chi_0)\rangle_j$ [$|\phi(\varphi_0, \zeta_0)\rangle_j$ and $|\phi(\varphi_0 + \pi, \zeta_0)\rangle_j$] of the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ are degenerate, the phases θ_0 and χ_0 (φ_0 and ζ_0) are not fixed. For example, if the intra-dimer Hamiltonian contains only the XXZ exchange term, i.e., if $K_d = D_d = H_d^{\text{uni}} = H_d^{\text{sig}} = 0$ in Eq. (4), the eigenstates $|\phi(\varphi_0, \zeta_0)\rangle_j$ and $|\phi(\varphi_0 + \pi, \zeta_0)\rangle_j$ are degenerate irrespective of the values of J_d and Δ_d . If this is the case, the phases φ_0 and ζ_0 are not fixed, and the product state $\prod_j |\phi(\varphi_0, \zeta_0)\rangle_j$ with arbitrary φ_0 and ζ_0 is an eigenstate of the whole Hamiltonian. Such degenerate eigenstates was found in the model in one-dimensional lattice²⁶.

It can be proven in the following way that the eigenstates obtained above become the ground states of the whole Hamiltonian in some parameter regions. For instance, we consider the case of the inter-dimer Hamiltonian (31) with $\tilde{J}_{+-} = \tilde{J}_{-+}$ [Fig. 2 (b)] and the product state $\prod_j |\psi(\theta_j, \chi_j)\rangle_j$. To prove that the state can be the ground state, it is convenient to consider the intra-dimer Hamiltonian first. Let us assume that $|\psi(\theta_0, \chi_0)\rangle_j$ is the lowest-energy eigenstate of the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ and is not degenerate to the other three eigenstates. In this case, the ground state of the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ for the whole system is the product state $\prod_j |\psi(\theta_0, \chi_0)\rangle_j$ and there is a finite energy gap E_{gap} to the first excited states [see Fig. 3 (a)]. The ground state is unique while the first excited states are degenerate massively (N -fold or more, where N is the number of dimer units in the system). When the inter-dimer Hamiltonian $\mathcal{H}_{\text{inter}}$ is included, the ground state as well as its energy is unchanged since the state is an eigenstate of $\mathcal{H}_{\text{inter}}$ with the zero eigenvalue. On the

TABLE I: Outcomes of the inter-dimer exchange couplings acting on the two-dimer product states. Equations in the table show the condition required for having zero as the resultant state. Here, $|s\rangle_k$ and $|t_0\rangle_k$ ($k = j, j'$) denote the dimer-singlet state [Eq. (35)] and the dimer-triplet state with zero magnetization [Eq. (37)], respectively. The symbol “0” means that the resultant state is zero irrespective of the phases of the state considered, while “-” represents the case where the resultant state is not zero for any values of the phases.

	$ \psi(\theta_j, \chi_j)\rangle_j \psi(\theta_{j'}, \chi_{j'})\rangle_{j'}$	$ \phi(\varphi_j, \zeta_j)\rangle_j \phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$	$ \psi(\theta_j, \chi_j)\rangle_j \phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$	$ \phi(\varphi_j, \zeta_j)\rangle_j \psi(\theta_{j'}, \chi_{j'})\rangle_{j'}$
$h_{+-}^{XY}(j, j')$	$ \psi\rangle_j = s\rangle_j$ or $ \psi\rangle_{j'} = t_0\rangle_{j'}$	$\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	$ \psi\rangle_j = s\rangle_j$	$ \psi\rangle_{j'} = t_0\rangle_{j'}$
$h_{+-}^{\text{Ising}}(j, j')$	0	0	0	-
$h_{-+}^{XY}(j, j')$	$ \psi\rangle_j = t_0\rangle_j$ or $ \psi\rangle_{j'} = s\rangle_{j'}$	$\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	$ \psi\rangle_j = t_0\rangle_j$	$ \psi\rangle_{j'} = s\rangle_{j'}$
$h_{-+}^{\text{Ising}}(j, j')$	0	0	-	0
$h_{++}^{XY}(j, j') + h_{--}^{XY}(j, j')$	$\theta_j = \theta_{j'}$ and $\chi_j = \chi_{j'}$	$\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	-	-
$h_{++}^{\text{Ising}}(j, j') + h_{--}^{\text{Ising}}(j, j')$	0	0	-	-
$h_{+-}^{XY}(j, j')$	$ \psi\rangle_j = s\rangle_j$ or $ \psi\rangle_{j'} = s\rangle_{j'}$	$\varphi_j = -\varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	$ \psi\rangle_j = s\rangle_j$	$ \psi\rangle_{j'} = s\rangle_{j'}$
$h_{+-}^{\text{Ising}}(j, j')$	0	-	0	0
$h_{-+}^{XY}(j, j')$	$ \psi\rangle_j = t_0\rangle_j$ or $ \psi\rangle_{j'} = t_0\rangle_{j'}$	$\varphi_j = -\varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	$ \psi\rangle_j = t_0\rangle_j$	$ \psi\rangle_{j'} = t_0\rangle_{j'}$
$h_{-+}^{\text{Ising}}(j, j')$	-	0	0	0
$h_{++}^{XY}(j, j') + h_{--}^{XY}(j, j')$	$\theta_j = -\theta_{j'}$ and $\chi_j = \chi_{j'}$	$\varphi_j = -\varphi_{j'}$ and $\zeta_j = \zeta_{j'}$	-	-
$h_{++}^{\text{Ising}}(j, j') + h_{--}^{\text{Ising}}(j, j')$	-	-	0	0

other hand, the excited states are modified by the inter-dimer Hamiltonian and the manifold of the first-excited states forms an energy band. The “band width” should be of the order of the energy scale of the inter-dimer Hamiltonian. Therefore, if the energy gap E_{gap} is larger than a critical value which has the same order as the energy scale of the inter-dimer Hamiltonian, the product state $\prod_j |\psi(\theta_0, \chi_0)\rangle_j$ remains as the ground state of the whole Hamiltonian. We thereby obtain the exact ground state. We note that such an exact ground state was found in the case of one-dimensional lattice in Refs. 25 and 26. In these studies, the Hamiltonian (31) with $\tilde{J}_{+-} = \tilde{J}_{-+}$ [Eq. (2) with $J_{11} = -J_{22}$ and $J_{21} = J_{12} = 0$, see Fig. 2 (b)] was considered for the inter-dimer Hamiltonian, while the intra-dimer Hamiltonian (4) is assumed to contain the XXZ exchange term only [$K_d = D_d = H_d^{\text{uni}} = H_d^{\text{sg}} = 0$]. It was found²⁵ that the model with $\Delta = \Delta_d = 1$ and $J_d > 1.134461J_{11}$ has the product state of the dimer-singlet,

$$|\text{DS}\rangle = \prod_j |s\rangle_j, \quad (34)$$

$$|s\rangle_j = \left| \psi\left(\frac{3\pi}{2}, 0\right) \right\rangle_j = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_j - |\downarrow\uparrow\rangle_j), \quad (35)$$

as the exact ground state. It was also reported²⁶ that the model with $J_{11} = -J_{22} = 0.2$, $\Delta = 1$, $J_d = -1$, and $0 \leq \Delta_d \leq 0.83$ has the product state of the dimer-triplet with zero magnetization,

$$|\text{DT}_0\rangle = \prod_j |t_0\rangle_j, \quad (36)$$

$$|t_0\rangle_j = \left| \psi\left(\frac{\pi}{2}, 0\right) \right\rangle_j = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_j + |\downarrow\uparrow\rangle_j), \quad (37)$$

as the exact ground state.

Finally, we discuss the case where the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ has degenerate ground states, choosing, as an example, the case where the states $|\phi(\varphi_0, \zeta_0)\rangle_j$ and

$|\phi(\varphi_0 + \pi, \zeta_0)\rangle_j$ are the doubly-degenerate ground states of $h_{\text{intra}}(j)$. (Here, the values of φ_0 and ζ_0 can be taken arbitrarily.) This indeed occurs when $h_{\text{intra}}(j)$ contains only the XXZ exchange term with $J_d < 0$ and $\Delta_d > 1$ (i.e., the exchange coupling is ferromagnetic and has the Ising anisotropy). In this case, the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ has 2^N -fold degenerate ground states; the Hilbert space of the ground-state manifold can be expanded by the product states $\prod_j |\phi(\varphi_j, 0)\rangle_j$ with φ_j taking one of the two values $\{\varphi_0, \varphi_0 + \pi\}$ arbitrarily. (Note that we can take $\zeta_j = 0$ without loss of generality.) When the inter-dimer Hamiltonian is included, this 2^N -fold degeneracy of the ground states is lifted: Although two out of the degenerate ground states of $\mathcal{H}_{\text{intra}}$, $\prod_j |\phi(\varphi_0, 0)\rangle_j$ and $\prod_j |\phi(\varphi_0 + \pi, 0)\rangle_j$ (the product states with uniform φ_j), remain the eigenstates, the other states are mixed by the inter-dimer Hamiltonian and form the energy band [see Fig. 3 (b)]. As a result, the ground state of the whole Hamiltonian is not a simple product of dimer states but becomes a complicated many-body state. We note that, if the anisotropic exchange coupling K_d is present in the intra-dimer Hamiltonian, the ground state of $\mathcal{H}_{\text{intra}}$ becomes unique. Then, if the energy gap to the first excited states is large enough, a product of dimer-spin-nematic states,

$$|\text{DN}(\varphi_0, \zeta_0)\rangle = \prod_j |\phi(\varphi_0, \zeta_0)\rangle_j, \quad (38)$$

where φ_0 and ζ_0 are fixed according to $\mathcal{H}_{\text{intra}}$, becomes the exact ground state of the whole Hamiltonian. It should be noticed that this spin-nematic state is not a result of a spontaneous symmetry breaking but due to the explicit anisotropy in the Hamiltonian.

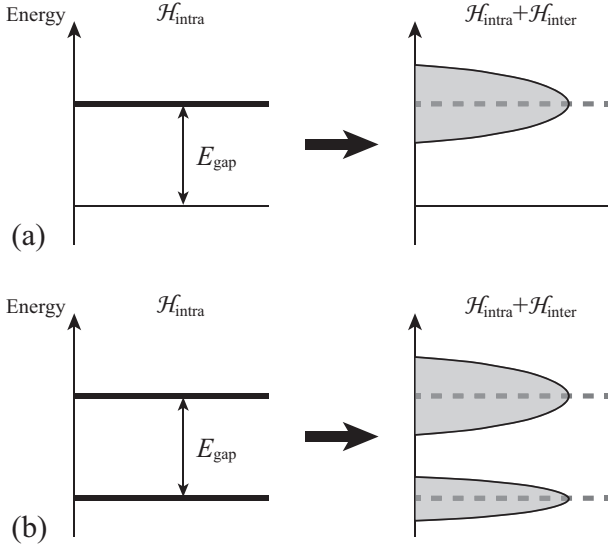


FIG. 3: Schematic pictures of the density of states. Thin and bold lines represent unique and degenerate energy levels, respectively. (a) The case where the ground state of the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ is unique. When the inter-dimer Hamiltonian $\mathcal{H}_{\text{inter}}$ is included, the ground state remains unchanged, while the first-excited states of $\mathcal{H}_{\text{intra}}$, which are massively degenerate, acquire a “kinetic energy” by $\mathcal{H}_{\text{inter}}$ and form an energy band. (b) The case where the ground states of $\mathcal{H}_{\text{intra}}$ are also degenerate. In this case, not only the manifolds of the excited states but also the manifold of the ground states form an energy band at the inclusion of $\mathcal{H}_{\text{inter}}$, and the eigenstate of $\mathcal{H}_{\text{intra}}$ is not the ground state of the whole Hamiltonian $\mathcal{H}_{\text{inter}} + \mathcal{H}_{\text{intra}}$.

C. Example II of exact ground states

We discuss another example of the model having an exact ground state. The model considered consists of the inter-dimer Hamiltonian of the form,

$$\mathcal{H}_{\text{inter}} = \sum_{\langle j,j' \rangle} \left\{ \tilde{J}_{++} \left[h_{++}^{XY}(j,j') + \Delta h_{++}^{\text{Ising}}(j,j') \right] + \tilde{J}_{--} \left[h_{--}^{XY}(j,j') + \Delta h_{--}^{\text{Ising}}(j,j') \right] \right\}, \quad (39)$$

and the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ [Eq. (4)]. We consider the three parameter regions for the inter-dimer Hamiltonian:

- (a) $\tilde{J}_{++} = 0$: In this case, the inter-dimer Hamiltonian is given by Eq. (2) with $J_{11} = J_{22} = -J_{12} = -J_{21} = \tilde{J}_{--}$ [Fig. 4 (a)].
- (b) $\Delta = 0$: The exchange couplings in the inter-dimer Hamiltonian is of the XY-type and the exchange coupling constants in Eq. (2) obey the relation $J_{11} = J_{22} = \tilde{J}_{++} + \tilde{J}_{--}$ and $J_{12} = J_{21} = \tilde{J}_{++} - \tilde{J}_{--}$ [Fig. 4 (b)].
- (c) $\tilde{J}_{++} = \tilde{J}_{--}$ and $\Delta = 0$: The inter-dimer exchanges are of the XY-type and the coupling constants in Eq. (2) obey $J_{11} = J_{22} = \tilde{J}_{++} + \tilde{J}_{--}$ and $J_{12} = J_{21} = 0$ [Fig. 4 (c)]. This is a special case of the model (b) above.

We also assume that the lattice is bipartite and the coupling constants in the intra-dimer Hamiltonian (4) take one of two

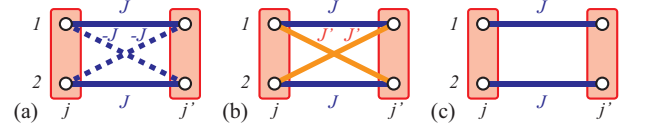


FIG. 4: Schematic pictures of (a) the inter-dimer Hamiltonian (39) with $\tilde{J}_{++} = 0$, where $J = \tilde{J}_{--}$, (b) the inter-dimer Hamiltonian (39), where $J = \tilde{J}_{++} + \tilde{J}_{--}$ and $J' = \tilde{J}_{++} - \tilde{J}_{--}$, and (c) the same Hamiltonian as (b) with $\tilde{J}_{++} = \tilde{J}_{--}$. For the models (b) and (c), the XY case ($\Delta = 0$) is considered in the text.

values depending on the sublattice A or B, i.e., $J_d(j) = J_{d,A}$ ($j \in A$), $J_{d,B}$ ($j \in B$), and so on.

We can find the parameter region of the model with an exact ground state in the same manner as described in the previous section. From the results in Table I, it follows that in all of the three cases listed above, the inter-dimer Hamiltonian has the product state,

$$\prod_{j \in A} |\phi(\varphi, \zeta)\rangle_j \prod_{j \in B} |\phi(-\varphi, \zeta)\rangle_j, \quad (40)$$

with arbitrary φ and ζ as an eigenstate with zero eigenvalue. Then, if the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ in sublattices A and B has respectively the states $|\phi(\varphi_0, \zeta_0)\rangle_j$ and $|\phi(-\varphi_0, \zeta_0)\rangle_j$ with certain φ_0 and ζ_0 as an eigenstate, the product state (40) with $\varphi = \varphi_0$ and $\zeta = \zeta_0$ is an eigenstate of the whole Hamiltonian. We note that such staggered $\varphi_j = \pm\varphi_0$ and uniform $\zeta_j = \zeta_0$ can be realized by taking the coupling constant of the anisotropic exchange terms $h^{\text{ani}}(j)$ in the staggered way, $K_d(j) = K_{d,A} < 0$ ($j \in A$), $K_{d,B} > 0$ ($j \in B$) and setting $\eta_d(j) = H^{\text{uni}}(j) = 0$ in the intra-dimer Hamiltonian. In this case, the product state,

$$\begin{aligned} & \prod_{j \in A} \left| \phi\left(\frac{\pi}{2}, 0\right) \right\rangle_j \prod_{j \in B} \left| \phi\left(-\frac{\pi}{2}, 0\right) \right\rangle_j \\ &= \prod_{j \in A} \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle_j + |\downarrow\downarrow\rangle_j) \prod_{j \in B} \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle_j - |\downarrow\downarrow\rangle_j), \end{aligned} \quad (41)$$

is the eigenstate of the whole Hamiltonian. Finally, if the product state is the ground state of the intra-dimer Hamiltonian $\mathcal{H}_{\text{intra}}$ with a sufficiently large excitation gap, the state becomes the exact ground state of the whole Hamiltonian $\mathcal{H}_{\text{inter}} + \mathcal{H}_{\text{intra}}$.

We also see in Table I that the inter-dimer Hamiltonian in the case (c) mentioned above has the product state,

$$\prod_{j \in A} |\psi(\theta, \chi)\rangle_j \prod_{j \in B} |\psi(-\theta, \chi)\rangle_j, \quad (42)$$

with arbitrary θ and χ as an eigenstate with zero eigenvalue. Then, if the intra-dimer Hamiltonian has the product state (42) with $\theta = \theta_0$ and $\chi = \chi_0$ as the ground state with a sufficiently large excitation gap, the product state becomes the exact ground state of the whole Hamiltonian. The staggered $\theta_j = \pm\theta_0$ and uniform $\chi_j = \chi_0$ of the ground state can be realized in a rather simple way: If the intra-dimer Hamiltonian

contains only the XXZ exchange terms with $J_d(j) = J_d > 0$ (antiferromagnetic) for $j \in A$ and $J_d(j) = J'_d < 0$ and $0 \leq \Delta_d(j) < 1$ (ferromagnetic and XY -like anisotropic) for $j \in B$, the product state,

$$\begin{aligned} & \prod_{j \in A} \left| \psi \left(-\frac{\pi}{2}, 0 \right) \right\rangle_j \prod_{j \in B} \left| \psi \left(\frac{\pi}{2}, 0 \right) \right\rangle_j \\ &= \prod_{j \in A} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_j - |\downarrow\uparrow\rangle_j) \prod_{j \in B} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle_j + |\downarrow\uparrow\rangle_j) \\ &= \prod_{j \in A} |s\rangle_j \prod_{j \in B} |t_0\rangle_j, \end{aligned} \quad (43)$$

is the ground state of the intra-dimer Hamiltonian. This product state becomes the exact ground state of the whole Hamiltonian if the intra-dimer exchange constants J_d and $|J'_d|$ are sufficiently large. We thereby find the model with the exact ground state in which the dimer-singlet state and the dimer-triplet state with zero magnetization are arranged in a staggered fashion. We note that when $\Delta_d = 0$ (i.e., not only the inter-dimer exchange couplings but also the intra-dimer ones are of the XY type), the model and the ground state [Eq. (43)] considered here are connected to the models and the states [Eq. (35) and (37)] discussed in the previous section through unitary transformations of the spin rotation.

D. Other examples

In addition to the cases discussed in the preceding sections, we see in Table I many cases where the outcome of $h_{\epsilon\epsilon'}^{XY}(j, j')$ acting on the two-dimer product state is zero. Namely,

$$h_{\epsilon\epsilon'}^{XY}(j, j') |f\rangle_j |f'\rangle_{j'} = 0, \quad (44)$$

when $\epsilon (\epsilon') = +$ and $|f\rangle_j = |s\rangle_j$ ($|f'\rangle_{j'} = |s\rangle_{j'}$), or $\epsilon (\epsilon') = -$ and $|f\rangle_j = |t_0\rangle_j$ ($|f'\rangle_{j'} = |t_0\rangle_{j'}$). This comes from the fact that $S_{1,j}^\pm + S_{2,j}^\pm$ ($S_{1,j}^\pm - S_{2,j}^\pm$) acting on $|s\rangle_j$ ($|t_0\rangle_j$) yields zero,

$$(S_{1,j}^\pm + S_{2,j}^\pm) |s\rangle_j = (S_{1,j}^\pm - S_{2,j}^\pm) |t_0\rangle_j = 0. \quad (45)$$

A simple example of the application of Eq. (44) can be found in the model consisting of the inter-dimer Hamiltonian,

$$\mathcal{H}_{\text{inter}} = \sum_{\langle j, j' \rangle} \tilde{J}_{++} [h_{++}^{XY}(j, j') + \Delta h_{++}^{\text{Ising}}(j, j')], \quad (46)$$

and the intra-dimer Hamiltonian including only the XXZ exchange couplings. For this model, the product state of the dimer-singlet states, $|DS\rangle$ [Eq. (34)], is the exact eigenstate of $\mathcal{H}_{\text{inter}}$ with zero eigenvalue and becomes the exact ground state of the whole Hamiltonian if the XXZ exchange couplings in the intra-dimer Hamiltonian are antiferromagnetic and sufficiently strong. We note that this mechanism to realize the dimer-singlet-product ground state can be understood from the viewpoint that $(S_{1,j} + S_{2,j})^2$ for each dimer unit is a good quantum number in the model. This type of the exact ground state has been reported for various frustrated spin models^{19–21,24}.

Equation (44) can be used to derive many other models with an exact ground state. Let us consider, for instance, the inter-dimer Hamiltonian,

$$\mathcal{H}_{\text{inter}} = \sum_{\langle j, j' \rangle} \tilde{J}_{--} [h_{--}^{XY}(j, j') + \Delta h_{--}^{\text{Ising}}(j, j')], \quad (47)$$

in a bipartite lattice. It is then found that the product state,

$$\prod_{j \in A} |t_0\rangle_j \prod_{j \in B} |\phi(\varphi_j, \zeta_j)\rangle_j, \quad (48)$$

is the eigenstate of $\mathcal{H}_{\text{inter}}$ with zero eigenvalue. Therefore, if the local intra-dimer Hamiltonian $h_{\text{intra}}(j)$ in sublattice A has $|t_0\rangle_j$ as an eigenstate and $h_{\text{intra}}(j)$ in sublattice B does the spin-nematic state $|\phi(\varphi_0, \zeta_0)\rangle_j$ (with certain φ_0 and ζ_0), the product state $\prod_{j \in A} |t_0\rangle_j \prod_{j \in B} |\phi(\varphi_0, \zeta_0)\rangle_j$ is the eigenstate of the whole Hamiltonian. Furthermore, if the excitation gap of the intra-dimer Hamiltonian is large enough, the product state becomes the exact ground state of the whole Hamiltonian. In such a manner, we can construct several models having an exact ground state written as a direct product of the dimer-singlet state $|s\rangle_j$, the dimer-triplet state with zero magnetization $|t_0\rangle_j$, and the spin-nematic state $|\phi(\varphi_0, \zeta_0)\rangle_j$.

IV. SUMMARY

In summary, we have studied frustrated quantum spin systems consisting of spin-dimer units, Eq. (1). We have shown that the systems in certain parameter regions has an exact ground state written in the form of direct product of dimer states. In the argument, we first specified the inter-dimer Hamiltonian which has the product state considered as an eigenstate with zero eigenvalue, and showed that the state can be the eigenstate of a certain intra-dimer Hamiltonian simultaneously. We then showed that the eigenstate becomes an exact ground state of the whole Hamiltonian (the sum of the inter- and intra-dimer Hamiltonian) when the coupling parameters in the intra-dimer Hamiltonian are selected appropriately. In such a way, we have found several models each of which has the exact ground state of the form of product of dimer states, including the product of the dimer-singlet states [Eq. (34)], that of the dimer-triplet states with zero magnetization [Eq. (36)], those of the dimer-spin-nematic states [Eq. (38)], and various products with two-sublattice structure. We have also introduced two operators $T_{1,j}$ and $T_{2,j}$ [Eqs. (10) and (11)]: The operator $T_{1,j}$ ($T_{2,j}$) acts in the subspace $\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$ ($\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$) as a spin-1/2 operator, while it is zero in the subspace $\{|\uparrow\uparrow\rangle_j, |\downarrow\downarrow\rangle_j\}$ ($\{|\uparrow\downarrow\rangle_j, |\downarrow\uparrow\rangle_j\}$).

Acknowledgments

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Appendix A

The cases where the inter-dimer exchange terms $h_{\epsilon\epsilon'}^{XY}(j, j')$ and $h_{\epsilon\epsilon'}^{\text{Ising}}(j, j')$ acting on a two-dimer product state give zero, which are summarized in Table I, can be divided into the following three groups.

First, the Ising terms $h_{\epsilon\epsilon'}^{\text{Ising}}(j, j')$ can be written in terms of $T_{1,k}^z$ and $T_{2,k}^z$ ($k = j, j'$) as mentioned in Sect. III A. Therefore, when $h_{\epsilon\epsilon'}^{\text{Ising}}(j, j')$ including $T_{1,k}^z$ [$T_{2,k}^z$] acts on $|\psi(\theta_k, \chi_k)\rangle_k$ [$|\phi(\varphi_k, \zeta_k)\rangle_k$], the outcome is zero. These cases are listed as “0” in Table I.

Second, it follows from Eq. (45) that the XY terms $h_{\epsilon\epsilon'}^{XY}(j, j')$ including the factor $(S_{1,k}^{\pm} + S_{2,k}^{\pm}) [(S_{1,k}^{\pm} - S_{2,k}^{\pm})]$ yield zero when acting on the dimer-singlet state $|s\rangle_k$ [the dimer-triplet state with zero magnetization, $|t_0\rangle_k$]. These cases are listed in Table I as “ $|\psi\rangle_j = |s\rangle_j$ ”, “ $|\psi\rangle_j = |t_0\rangle_j$ ”, and so on.

Third, there are other non-trivial cases where the XY terms $h_{\epsilon\epsilon'}^{XY}(j, j')$ yield zero. For instance, the outcome of $h_{+-}^{XY}(j, j')$ acting on $|\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$ is given by

$$\begin{aligned} & h_{+-}^{XY}(j, j') |\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'} \\ &= -\frac{1}{2} \left[\cos\left(\frac{\zeta_j - \zeta_{j'}}{2}\right) \sin\left(\frac{\varphi_j - \varphi_{j'}}{2}\right) \right. \\ & \quad \left. + i \sin\left(\frac{\zeta_j - \zeta_{j'}}{2}\right) \sin\left(\frac{\varphi_j + \varphi_{j'}}{2}\right) \right] \\ & \quad \times (|\uparrow\downarrow\rangle_j + |\downarrow\uparrow\rangle_j) (|\uparrow\downarrow\rangle_{j'} - |\downarrow\uparrow\rangle_{j'}). \quad (\text{A1}) \end{aligned}$$

This resultant state becomes zero if $\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$. We note that the state (A1) is zero also in the case of $\varphi_j = -\varphi_{j'}$ and $\zeta_j = \zeta_{j'} + \pi$. In our argument, we consider only the case of $\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$ since these two cases give the same state $|\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'}$ up to an overall factor. In addition, the state (A1) becomes zero for arbitrary ζ_j and $\zeta_{j'}$ if $\varphi_j = \varphi_{j'} = 0$ or $\varphi_j = \varphi_{j'} = \pi$. We ignore these cases of $\varphi_j = \varphi_{j'} = 0$ and $\varphi_j = \varphi_{j'} = \pi$ in our argument as they correspond to the trivial states $|\phi(\varphi_j, \zeta_j)\rangle_j |\phi(\varphi_{j'}, \zeta_{j'})\rangle_{j'} = |\uparrow\uparrow\rangle_j |\uparrow\uparrow\rangle_{j'}$ and $|\downarrow\downarrow\rangle_j |\downarrow\downarrow\rangle_{j'}$, respectively.

In a similar way, one can find that the outcome is zero for the cases denoted in Table I as “ $\theta_j = \theta_{j'}$ and $\chi_j = \chi_{j'}$ ”, “ $\varphi_j = \varphi_{j'}$ and $\zeta_j = \zeta_{j'}$ ”, “ $\theta_j = -\theta_{j'}$ and $\chi_j = \chi_{j'}$ ”, and “ $\varphi_j = -\varphi_{j'}$ and $\zeta_j = \zeta_{j'}$ ”. The zero states obtained in these cases stem from perfect destructive interferences among the inter-dimer exchange processes.

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